

# Orthogonal polynomial solutions to the non-central modified Kratzer potential

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## Abstract

We investigate the analytical solution of a new exactly solvable non-central potential of  $V(r, \theta) = D \left( \frac{r-a}{r} \right)^2 + \frac{\beta}{r^2 \sin^2 \theta} + \frac{\gamma \cos \theta}{r^2 \sin^2 \theta}$  type, which may be called as the modified non-central Kratzer potential. The energy eigenvalues as well as the corresponding eigenfunctions are calculated for various values of  $n$  and  $m$  quantum numbers within the framework of the Nikiforov-Uvarov and Asymptotic Iteration Methods for the  $CO$  diatomic molecule as an application of this potential. In this paper, we first present the effect of the non-central term on the bound-state energy eigenvalues: this effect is determined explicitly for different  $n$  and  $m$  quantum numbers with  $\beta = \gamma = 0.0, 0.1, 1.0$  and  $5.0$  values and the results are compared with the findings of the modified Kratzer potential for different  $n$  and  $l$  quantum numbers. Then, we show that the angle-dependent non-central part behaves like a centrifugal barrier and it reduces the depth of the attractive potential pocket, which effects the bound-state energy eigenvalues.

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## I. INTRODUCTION

The analytical solution of the radial Schrödinger equation is of high importance in non-relativistic quantum mechanics since the wave function contains all the necessary information to describe a quantum system fully. There are only a few potentials for which the radial Schrödinger equation can be solved explicitly for all  $n$  and all  $l$ . So far, many methods such as super-symmetry (SUSY) [1, 2, 3], Nikiforov-Uvarov [4, 5, 6, 7, 8], Asymptotic Iteration Method [9, 10, 11, 12, 13] and the Pekeris approximation [14, 15] have been developed and applied to solve the radial Schrödinger equation exactly or quasi-exactly for  $l \neq 0$  within a given potential.

The Kratzer or modified Kratzer type potentials [16] we consider in this paper have played an important role in the history of the molecular and quantum chemistry and they have been so far extensively used to describe the molecular structure and interactions [17]. Although such central potentials have been extensively used to describe the properties of the system qualitatively, it is known that the dynamical properties of the system should also be taken into account for a better description of the system. That means, the potential should have not only the radial but also the angle dependent parts. These dynamical properties of the system can be taken into account by using a non-central potential and therefore, in this paper, we aim to present the effect of the non-central term to calculate the non-zero angular momentum solutions of the Schrödinger equation. For this, we take the non-central modified Kratzer [18] potential  $(V(r, \theta) = D \left( \frac{r-a}{r} \right)^2 + \frac{\beta}{r^2 \sin^2 \theta} + \frac{\gamma \cos \theta}{r^2 \sin^2 \theta})$  and as an application, we calculate the energy eigenvalues of the *CO* diatomic molecule for various  $n$  and  $m$  quantum numbers.

The article is organized as follows: In the following two sections, the basic equations of the Nikiforov-Uvarov method (NU) as well as the Asymptotic Iteration Method (AIM) used so far to solve the resulting differential equation are given briefly. The solutions of the Schrödinger equation with the non-central modified Kratzer potential are outlined in the fourth section. Then, the solutions of the Schrödinger equation with the non-central modified Kratzer potential are obtained by using both methods. The energy eigenvalues and the corresponding eigenfunctions are calculated for various values of  $n$  and  $m$  quantum numbers for the *CO* diatomic molecule and the effect of the non-central term is determined explicitly by comparing the results with the findings of the modified Kratzer potential with different

$n$  and  $l$  quantum numbers. The summary and conclusion are provided in section VII.

## II. NIKIFOROV-UVAROV METHOD

The NU method is based on the solutions of general second order linear equations with special functions. It has been extensively used to solve the non-relativistic Schrödinger equation or similar time-independent second-order differential equations and there is an extensive literature to look at [4, 5, 6, 7, 8]. However, in order to keep the completeness of the paper, we briefly outline NU method here. The idea in the NU method is to convert the Schrödinger equation or similar differential equations into the following form:

$$\psi(s)'' + \frac{\tilde{\tau}(s)}{\sigma(s)}\psi'(s) + \frac{\tilde{\sigma}(s)}{\sigma^2(s)}\psi(s) = 0 \quad (1)$$

where  $\sigma(s)$  and  $\tilde{\sigma}(s)$  are polynomials, at most second-degree, and  $\tilde{\tau}(s)$  is a first-degree polynomial [4, 5, 6, 7, 8]. Hence, from Eq. (1), the Schrödinger equation or the Schrödinger-like equations can be solved analytically by this method. In order to find a particular solution of Eq. (1), the following transformation is used:

$$\psi(s) = \phi(s)y(s) \quad (2)$$

it reduces Eq. (1) to an equation of hypergeometric type,

$$\sigma(s)y'' + \tau(s)y' + \lambda y = 0 \quad (3)$$

and  $\phi(s)$  is defined as a logarithmic derivative in the following form and its solutions can be obtained from

$$\phi'(s)/\phi(s) = \pi(s)/\sigma(s) \quad (4)$$

The other part  $y(s)$  is the hypergeometric type function whose polynomial solutions are given by the Rodrigues relation

$$y_n(s) = \frac{B_n}{\rho(s)} \frac{d^n}{ds^n} [\sigma^n(s)\rho(s)] \quad (5)$$

where  $B_n$  is the normalization constant and the weight function  $\rho(s)$  must satisfy the condition

$$(\sigma\rho)' = \tau\rho \quad (6)$$

The function  $\pi$  and the parameter  $\lambda$  required for this method are defined as follows

$$\pi(s) = \frac{\sigma' - \tilde{\tau}}{2} \pm \sqrt{\left(\frac{\sigma' - \tilde{\tau}}{2}\right)^2 - \tilde{\sigma} + k\sigma} \quad , \quad (7)$$

$$\lambda = k + \pi' \quad (8)$$

On the other hand, in order to find the value of  $k$ , the expression under the square root must be the square of a polynomial. Thus, a new eigenvalue equation for the Schrödinger equation becomes

$$\lambda = \lambda_n = -n\tau' - \frac{n(n-1)}{2}\sigma'' \quad (9)$$

where

$$\tau(s) = \tilde{\tau}(s) + 2\pi(s) \quad (10)$$

and its derivative is negative. By comparison of Eqs. (8) and (9), we obtain the energy eigenvalues.

### III. THE ASYMPTOTIC ITERATION METHOD (AIM)

In this section we briefly outline the asymptotic iteration method, the details can be found in references [9, 10, 11, 12, 13]. The asymptotic iteration method was proposed to solve second-order differential equations of the form

$$y'' = \lambda_0(x)y' + s_0(x)y \quad (11)$$

where  $s_0(x)$ ,  $\lambda_0(x)$  are functions in  $C_\infty(a,b)$ . The variables,  $s_0(x)$  and  $\lambda_0(x)$ , are sufficiently differentiable.

$$y''' = \lambda_1(x)y' + s_1(x)y \quad (12)$$

The second derivative of Eq.(11) is obtained as

$$y'''' = \lambda_2(x)y' + s_2(x)y \quad (13)$$

where

$$\lambda_1(x) = \lambda_0'(x) + s_0(x) + \lambda_0^2(x) \quad s_1(x) = s_0'(x) + s_0(x)\lambda_0(x)$$

$$\lambda_2(x) = \lambda_1'(x) + s_1(x) + \lambda_0(x)\lambda_1 \quad s_2(x) = s_1'(x) + s_0(x)\lambda_1(x) \quad (14)$$

Therefore, for  $(n+1)^{th}$  and  $(n+2)^{th}$  derivatives,  $n=1,2,\dots$ , one can get,

$$y^{(n+1)} = \lambda_{n-1}(x)y' + s_{n-1}(x)y \quad (15)$$

and

$$y^{(n+2)} = \lambda_n(x)y' + s_n(x)y \quad (16)$$

respectively, where

$$\lambda_n(x) = \lambda_{n-1}'(x) + s_{n-1}(x) + \lambda_0(x)\lambda_{n-1}(x) \quad s_n(x) = s_{n-1}'(x) + s_0(x)\lambda_{n-1}(x) \quad (17)$$

The ratio of the  $(n+2)^{th}$  and  $(n+1)^{th}$  derivatives can be expressed as

$$\frac{d}{dx} \ln(y^{(n+1)}) = \frac{y^{(n+2)}}{y^{(n+1)}} = \frac{\lambda_n(y' + \frac{s_n}{\lambda_n}y)}{\lambda_{n-1}(y' + \frac{s_{n-1}}{\lambda_{n-1}}y)} \quad (18)$$

For sufficiently large  $n$ , we can now introduce the asymptotic aspect of the method; that is,

$$\frac{s_n}{\lambda_n} = \frac{s_{n-1}}{\lambda_{n-1}} = \alpha \quad (19)$$

Thus Eq.(18) can be reduced to

$$\frac{d}{dx} \ln(y^{(n+1)}) = \frac{\lambda_n}{\lambda_{n-1}} \quad (20)$$

which yields the general solution of Eq.(11) [9]

$$y(x) = \exp\left(-\int^x \alpha dt\right) \left[ C_2 + C_1 \int^x \exp\left(\int^t \lambda_0(\tau) + 2\alpha(\tau) d\tau\right) dt \right] \quad (21)$$

For a given potential such as non-central modified Kratzer, Schrödinger equations are converted to the form of Eq.(11). Then,  $s_0(x)$  and  $\lambda_0(x)$  are determined and  $s_n(x)$  and  $\lambda_n(x)$  parameters are calculated. The energy eigenvalues are obtained by the termination condition given by Eq.(19).

In this study, we investigate the exact solutions of the Schrödinger equations which the relevant second order homogenous linear differential equation takes the following general form [10],

$$y'' = 2 \left( \frac{ax^{N+1}}{1-bx^{N+2}} - \frac{(m+1)}{x} \right) y' - \frac{wx^N}{1-bx^{N+2}} y \quad (22)$$

If this equation is compared to Eq.(11), it entails the following expressions

$$\lambda_0(x) = 2 \left( \frac{ax^{N+1}}{1-bx^{N+2}} - \frac{(m+1)}{x} \right) \quad s_0(x) = -\frac{wx^N}{1-bx^{N+2}} \quad (23)$$

$a$ ,  $b$  and  $m$  are real numbers and  $w_n^m(N)$  can be determined from condition Eq.(19) as follows

$$w_n^m(-1) = n(2a + 2bm + (n+1)b) \quad (24)$$

$$w_n^m(0) = 2n(2a + 2bm + (2n+1)b) \quad (25)$$

$$w_n^m(1) = 3n(2a + 2bm + (3n+1)b) \quad (26)$$

$$w_n^m(2) = 4n(2a + 2bm + (4n+1)b) \quad (27)$$

$$w_n^m(3) = 5n(2a + 2bm + (5n+1)b) \quad (28)$$

... etc

Hence, these formulae are easily generalized as;

$$w_n^m(N) = b(N+2)^2 n \left( n + \frac{(2m+1)b + 2a}{(N+2)b} \right) \quad (29)$$

where  $n = 0, 1, 2, 3, \dots$  and  $N = -1, 0, 1, 2, 3, \dots$ . The exact eigenfunctions can be derived from the following generator:

$$y_n(x) = C_2 \exp \left( - \int^x \alpha_k dt \right) \quad (30)$$

where  $n = 0, 1, 2, \dots$  and  $k \geq n$  is the iteration step number. Using termination condition of the method given by Eq.(19) and  $\lambda_0$  and  $s_0$  determined by Eq.(23), the eigenfunctions are obtained as follows;

$$\begin{aligned} y_0(x) &= 1 \\ y_1(x) &= -C_2(N+2)\sigma \left( 1 - \frac{b(\rho+1)}{\sigma} x^{N+2} \right) \\ y_2(x) &= C_2(N+2)^2\sigma(\sigma+1) \left( 1 - \frac{2b(\rho+2)}{\sigma} x^{N+2} + \frac{b^2(\rho+2)(\rho+3)}{\sigma(\sigma+1)} x^{2(N+2)} \right) \\ y_3(x) &= -C_2 \frac{\sigma(\sigma+1)(\sigma+2)}{(N+2)^{-3}} \left( 1 - \frac{3b(\rho+3)}{\sigma} x^{N+2} \right. \\ &\quad \left. + \frac{3b^2(\rho+3)(\rho+4)}{\sigma(\sigma+1)} x^{2(N+2)} - \frac{b^3(\rho+3)(\rho+4)(\rho+5)}{\rho(\rho+1)(\rho+2)} x^{3(N+2)} \right) \\ &\dots etc \end{aligned}$$

Finally, the following general formula for the exact solutions  $y_n(x)$  is found as;

$$y_n(x) = (-1)^n C_2(N+2)^n (\sigma)_n {}_2F_1(-n, \rho+n; \sigma; bx^{N+2}) \quad (31)$$

where  $(\sigma)_n = \frac{\Gamma(\sigma+n)}{\Gamma(\sigma)}$ ,  $\sigma = \frac{2m+N+3}{N+2}$  and  $\rho = \frac{(2m+1)b+2a}{(N+2)b}$ .

#### IV. ENERGY EIGENVALUES USING NU METHOD

In this section, we show how to solve the Schrödinger equation for a particle in the presence of non-central modified Kratzer potential by using NU method. The standard Kratzer potential is defined by  $V(r) = -D \left( \frac{2a}{r} - \frac{a^2}{r^2} \right)$ . Similar to [8, 15, 18], the modified Kratzer potential is obtained by adding a D term to the standard Kratzer potential that is  $V(r) = D \left( \frac{r-a}{r} \right)^2$ . The new exactly solvable non-central modified Kratzer potential we examine in this paper is defined as follows:

$$V(r, \theta) = D \left( \frac{r-a}{r} \right)^2 + \frac{\beta}{r^2 \sin^2 \theta} + \frac{\gamma \cos \theta}{r^2 \sin^2 \theta} \quad (32)$$

where  $D$  is the dissociation energy and  $a$  is the equilibrium internuclear separation and  $\beta$  and  $\gamma$  are strictly positive constants [8, 15, 18]. The first term of this potential is the modified Kratzer potential, the second and third terms are the angle dependent parts. Thus, the non-central modified Kratzer potential is defined as a new potential. For the  $CO$  diatomic molecule, a comparison of the modified Kratzer and the non-central modified Kratzer potentials is shown in Figure 1 for different  $\beta$  and  $\gamma$  values with  $\theta = 30^\circ$  for the non-central part. The spectroscopic parameters of the  $CO$  diatomic molecule [19] are given in Table I.

In the spherical coordinates, the Schrödinger equation with the non-central modified Kratzer potential is

$$-\frac{\hbar^2}{2\mu} \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right] \psi + \left[ D \left( \frac{r-a}{r} \right)^2 + \frac{\beta}{r^2 \sin^2 \theta} + \frac{\gamma \cos \theta}{r^2 \sin^2 \theta} \right] \psi = E\psi \quad (33)$$

If the spherical total wavefunction as  $\psi(r, \theta, \varphi) = \frac{R(r)}{r} Y(\theta, \varphi) = U(r) Y(\theta, \varphi)$  is inserted into Eq. (33), the wave equation for the non-central modified Kratzer potential is separated into variables and the following equations are obtained:

$$\frac{d^2 R}{dr^2} + \frac{2\mu}{\hbar^2} \left[ E - D \left( \frac{r-a}{r} \right)^2 \right] R - \frac{\lambda}{r^2} R = 0 \quad (34)$$

$$\frac{d^2 \Theta(\theta)}{d\theta^2} + \cot \theta \frac{d\Theta(\theta)}{d\theta} + \left[ \lambda - \frac{m^2}{\sin^2 \theta} - \frac{2\mu}{\hbar^2} \left( \frac{\beta + \gamma \cos \theta}{\sin^2 \theta} \right) \right] \Theta(\theta) = 0 \quad (35)$$

$$\frac{d^2\Phi(\varphi)}{d\varphi^2} + m^2\Phi(\varphi) = 0 \quad (36)$$

where  $m^2$  and  $\lambda = l(l+1)$  are the separation constants. The solution of Eq. (36) is the well-known azimuthal angle solution. Eqs. (34) and (35) are the radial and the polar-angle equations. They have been examined separately in Refs. [7, 8]. In this paper, in order for the completeness of the paper, instead of just quoting their results and then discussing the effect of this new potential, we briefly show how to solve these equations by using the Nikiforov-Uvarov method [4] and then show the physical implications of this new non-central modified Kratzer potential. The radial part of the Schrödinger equation given by equation (34) can be written as

$$\frac{d^2R}{dr^2} + \frac{2\mu}{\hbar^2 r^2} \left[ (E - D)r^2 + 2Dar - \left( Da^2 + \frac{\lambda\hbar^2}{2\mu} \right) \right] R = 0 \quad (37)$$

This equation can be further arranged as

$$\frac{d^2R}{dr^2} + \frac{1}{r^2} (\varepsilon^2 r^2 - \xi r - \kappa) R = 0 \quad (38)$$

with the following abbreviations

$$\varepsilon^2 = \frac{2\mu(E - D)}{\hbar^2} ; \quad -\xi = \frac{4\mu Da}{\hbar^2} ; \quad \kappa = \frac{2\mu \left( Da^2 + \frac{\lambda\hbar^2}{2\mu} \right)}{\hbar^2} \quad (39)$$

It is now suitable for a NU solution. It is necessary to compare Eq. (38) with Eq. (1) to find the solution of this equation. When these equations are compared, we obtain the following polynomials:

$$\tilde{\tau}(r) = 0 \quad , \quad \sigma(r) = r \quad , \quad \tilde{\sigma}(r) = \varepsilon^2 r^2 - \xi r - \kappa \quad (40)$$

If these polynomials are inserted into Eq. (7), we get  $\pi$  function as

$$\pi = \frac{1}{2} \pm \sqrt{-4\varepsilon^2 r^2 + 4r(k + \xi) + 4\kappa + 1} \quad (41)$$

The expression in the square root must be the square of a polynomial according to the NU method. Thus, we can determine the constant  $k$  by using the condition that the discriminant of the square root is zero, that is,

$$k = -\xi \pm i\varepsilon\sqrt{1 + 4\kappa} \quad (42)$$



In view of that, new possible functions for each  $k$  are found as

$$\pi = \begin{cases} \frac{1}{2} \pm \frac{i}{2} [2r\varepsilon - i\sqrt{1+4\kappa}] & , \text{ for } k = -\xi + i\varepsilon\sqrt{1+4\kappa} \\ \frac{1}{2} \pm \frac{i}{2} [2r\varepsilon + i\sqrt{1+4\kappa}] & , \text{ for } k = -\xi - i\varepsilon\sqrt{1+4\kappa} \end{cases} \quad (43)$$

To obtain the negative derivative of  $\tau = \tilde{\tau} + 2\pi$ , we select

$$\pi(r) = \frac{1}{2} - \frac{i}{2} (2r\varepsilon + i\sqrt{1+4\kappa}) \quad (44)$$

and

$$k = -\xi - i\varepsilon\sqrt{1+4\kappa} \quad (45)$$

Using  $\lambda = k + \pi'$  together with the values  $k$  and  $\pi$ ,  $\tau$  and  $\lambda$  can be respectively obtained as

$$\tau(r) = 1 + \sqrt{1+4\kappa} - 2ir\varepsilon \quad (46)$$

$$\lambda = -\xi - i\varepsilon\sqrt{1+4\kappa} - i\varepsilon \quad (47)$$

Another definition of  $\lambda_n$  is given at Eq.(9),

$$\lambda_n = 2in\varepsilon \quad (48)$$

and comparing this with Eq.(47), the exact energy eigenvalues of the radial part of the Schrödinger equation with the non-central modified Kratzer potential are derived as

$$E_{nl} = D - \frac{8\mu D^2 a^2}{\hbar^2} \left( 1 + 2n + \sqrt{1 + 4 \left( \frac{2\mu D a^2}{\hbar^2} + l(l+1) \right)} \right)^{-2} \quad (49)$$

The energy eigenvalues calculated by this equation for the  $CO$  diatomic molecule are shown in the first column of Table II for different  $n$  and  $l$  values, which are in agreement with the results of Ref. [8].

It is also possible to determine the radial eigenfunction of this potential by considering Eq.(2) and using Eq.(4):

$$\phi(r) = r^{1/2(1+\sqrt{1+4\kappa})} e^{-i\varepsilon r} \quad (50)$$

From Eq. (5) and Eq. (6), we get

$$y(r) = \frac{B_{nl}}{\rho(r)} \frac{d^n}{dr^n} (r^n \rho(r)) \quad (51)$$

with  $\rho(r) = r^{\sqrt{1+4\kappa}} e^{-2i\varepsilon r}$ . If we get  $2i\varepsilon r = \zeta(r)$ ;  $\sqrt{1+4\kappa} = \nu$ , the  $R_{nl}$  radial wave function is

$$R_{nl}(\zeta) = B_{nl} \zeta^{1/2(1+\nu)} e^{-\zeta/2} L_n^\nu(\zeta) \quad (52)$$

if the definition of  $U_{nl}(r) = R_{nl}(r)/r$  is used, the total unnormalized radial wavefunction is

$$U_{nl}(\zeta) = B_{nl}\zeta^{-1/2(1-\nu)}e^{-\zeta/2}L_n^\nu(\zeta) \quad (53)$$

where  $B_{nl}$  is the normalization constant and it is evaluated as follows:

$$B_{nl} = \left( \frac{8\mu Da}{\hbar^2(2n + \nu + 1)} \right)^{3/2} \left[ \frac{n!}{(2n + \zeta + 1)(n + \zeta)!} \right]^{1/2} \quad (54)$$

For the non-central modified Kratzer potential, the angle dependent Schrödinger equation is given in Eq. (35). We may also derive the eigenvalues and eigenfunctions of the polar angle part of the Schrödinger equation [7] similar to the solutions of the radial part. We can write Eq. (35) by introducing a new variable [7],  $x = \cos \theta$ , as follows:

$$\frac{d^2\Theta(x)}{dx^2} - \frac{2x}{1-x^2} \frac{d\Theta(x)}{dx} + \left( \frac{\lambda(1-x^2) - m^2 - \frac{2\mu}{\hbar^2}(\beta + \gamma x)}{(1-x^2)^2} \right) \Theta(x) = 0 \quad (55)$$

To apply the Nikiforov-Uvarov method, Eq. (55) is compared with Eq. (1) and the following polynomials are obtained:

$$\tilde{\tau} = -2x, \quad \sigma = 1 - x^2, \quad \tilde{\sigma} = -\lambda x^2 - \frac{2\mu\gamma}{\hbar^2}x + \left( \lambda - m^2 - \frac{2\mu\beta}{\hbar^2} \right) \quad (56)$$

The function  $\pi$  is obtained by putting the above expression in Eq. (7),

$$\pi = \pm \sqrt{x^2(\lambda - k) + \frac{2\mu\gamma}{\hbar^2}x - (\lambda - m^2 - \frac{2\mu\beta}{\hbar^2} - k)} \quad (57)$$

Thus, the polynomial of  $\pi$  is found in four possible values:

$$\pi = \pm \begin{cases} x\sqrt{\frac{m^2 + \frac{2\mu\beta}{\hbar^2} + u}{2}} + \sqrt{\frac{m^2 + \frac{2\mu\beta}{\hbar^2} - u}{2}}, & \text{for } k = \frac{2\lambda - m^2 - \frac{2\mu\beta}{\hbar^2}}{2} - \frac{1}{2}u \\ x\sqrt{\frac{m^2 + \frac{2\mu\beta}{\hbar^2} - u}{2}} + \sqrt{\frac{m^2 + \frac{2\mu\beta}{\hbar^2} + u}{2}}, & \text{for } k = \frac{2\lambda - m^2 - \frac{2\mu\beta}{\hbar^2}}{2} + \frac{1}{2}u \end{cases} \quad (58)$$

where  $u = \sqrt{(m^2 + \frac{2\mu\beta}{\hbar^2})^2 - (\frac{2\mu\gamma}{\hbar^2})^2}$ . For the polynomial of  $\tau = \tilde{\tau} + 2\pi$  which has a negative derivative,

$$\tau = -2\sqrt{\frac{m^2 + \frac{2\mu\beta}{\hbar^2} - u}{2}} - 2x \left( 1 + \sqrt{\frac{m^2 + \frac{2\mu\beta}{\hbar^2} + u}{2}} \right) \quad (59)$$

Using Eq. (8) and Eq. (9), following expressions for the  $\lambda$  are obtained respectively

$$\lambda = \frac{2\lambda - (m^2 + \frac{2\mu\beta}{\hbar^2})}{2} - \frac{1}{2}u - \sqrt{\frac{m^2 + \frac{2\mu\beta}{\hbar^2} + u}{2}} \quad (60)$$

$$\lambda_n = 2n \left( 1 + \sqrt{\frac{m^2 + \frac{2\mu\beta}{h^2} + u}{2}} \right) + n(n-1) \quad (61)$$

If Eq. (60) and Eq. (61) are equated and the definition of  $\lambda = l(l+1)$  is used, the  $l$  values are obtained as

$$l = \sqrt{\frac{m^2 + \frac{2\mu\beta}{h^2} + \sqrt{(m^2 + \frac{2\mu\beta}{h^2})^2 - (\frac{2\mu\gamma}{h^2})^2}}{2}} + n \quad (62)$$

If these  $l$  values are inserted into the eigenvalues of the radial part of the Schrödinger equation with the non-central Kratzer potential given by Eq. (49), the energy eigenvalues are found as follows:

$$E_{nm} = D - \frac{8\mu D^2 a^2}{h^2} \times \left[ 1 + 2n + \sqrt{1 + 4 \left( \frac{2\mu D a^2}{h^2} + \left( \sqrt{\frac{m^2 + \frac{2\mu\beta}{h^2} + \sqrt{(m^2 + \frac{2\mu\beta}{h^2})^2 - (\frac{2\mu\gamma}{h^2})^2}}{2}} + n \right) \left( \sqrt{\frac{m^2 + \frac{2\mu\beta}{h^2} + \sqrt{(m^2 + \frac{2\mu\beta}{h^2})^2 - (\frac{2\mu\gamma}{h^2})^2}}{2}} + n + 1 \right) \right)} \right]^{-2} \quad (63)$$

We can also obtain the wave function of polar angle part of the Schrödinger equation [7], using  $\sigma$  and  $\pi$ ,

$$\phi(x) = (1-x)^{B+C/2} (1+x)^{B-C/2} \quad (64)$$

$$\rho(x) = (1-x^2)^B \left( \frac{1+x}{1-x} \right)^{-C} \quad (65)$$

$$y_n(x) = B_n (1-x)^{-(B+C)} (1+x)^{-(B-C)} \frac{d^n}{dx^n} \left[ (1+x)^{n+B-C} (1-x)^{n+B+C} \right] \quad (66)$$

where  $B = \sqrt{\frac{m^2 + \frac{2\mu\beta}{h^2} + u}{2}}$  and  $C = \sqrt{\frac{m^2 + \frac{2\mu\beta}{h^2} - u}{2}}$ . The polynomial solution of  $y_n$  is expressed in terms of Jacobi polynomials which are one of the orthogonal polynomials, giving  $\approx P_n^{(B+C, B-C)}(x)$ . The corresponding wave functions are found to be

$$\Theta_n(x) = N_n (1-x)^{(B+C)/2} (1+x)^{(B-C)/2} P_n^{(B+C, B-C)}(x) \quad (67)$$

where  $N_n$  is the normalization constant.

## V. ENERGY EIGENVALUES USING AIM

In this section, we show how to solve the Schrödinger equation for a particle in the presence of non-central modified Kratzer potential by using AIM. In the spherical coordinates,

the equation is given by

$$\left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} + \frac{2\mu}{\hbar^2} (E - V(r, \theta, \varphi)) \right] \psi(r, \theta, \varphi) = 0 \quad (68)$$

If one assigns the corresponding spherical total wave function as  $\psi(r, \theta, \varphi) = \frac{1}{r} R(r) Y(\theta, \varphi)$ , then by selecting  $Y(\theta, \varphi) = \frac{1}{\sin^{1/2} \theta} H(\theta) \Phi(\varphi)$ , the wave equation (68) for a general non-central potential is separated into variables and the following equations are obtained:

$$\frac{d^2 R(r)}{dr^2} + \left( \frac{2\mu}{\hbar^2} (E - V(r)) - \frac{l(l+1)}{r^2} \right) R(r) = 0 \quad (69)$$

$$\frac{d^2 H(\theta)}{d\theta^2} - \left( \frac{2\mu}{\hbar^2} V(\theta) + \frac{m^2}{\sin^2 \theta} - \frac{1}{2} - \frac{1 \cos^2 \theta}{4 \sin^2 \theta} - l(l+1) \right) H(\theta) = 0 \quad (70)$$

$$\frac{d^2 \Phi(\varphi)}{d\varphi^2} = -m^2 \Phi(\varphi) \quad (71)$$

where  $m^2$  and  $l(l+1)$  are separation constants. For bound states, we have the boundary conditions  $R(0)=0$  and  $R(\infty)=0$  in Eq.(69),  $H(0)$  and  $H(\pi)$  are infinite in Eq.(70) and  $\Phi(\varphi)=\Phi(\varphi+2\pi)$  in Eq.(71). If we specialize to the case where  $V(\varphi)=0$ , the normalized solution of the Eq.(71) that provides the boundary condition is

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \quad (m = 0, \pm 1, \pm 2, \dots) \quad (72)$$

In this section we consider solutions of radial and angle-dependent parts of Schrödinger equation for the non-central modified Kratzer potential within the framework of the asymptotic iteration method. The radial Schrödinger equation for the non-central modified Kratzer potential can be written as,

$$\frac{d^2 R(r)}{dr^2} + \left( \frac{2\mu}{\hbar^2} \left( E - D \left( 1 - \frac{2a}{r} + \frac{a^2}{r^2} \right) \right) - \frac{l(l+1)}{r^2} \right) R(r) = 0 \quad (73)$$

If the following abbreviations are used:

$$x = \frac{r}{a} \quad \epsilon^2 = -\frac{2\mu a^2}{\hbar^2} (E - D) \quad \alpha^2 = \frac{2\mu a^2}{\hbar^2} D \quad (74)$$

The radial Schrödinger equation takes the following form which is convenient in order to apply AIM.

$$\frac{d^2 R(x)}{dx^2} + \left( -\epsilon^2 + \frac{2\alpha^2}{x} - \frac{\alpha^2 + l(l+1)}{x^2} \right) R(x) = 0 \quad (75)$$

$$\frac{d^2 R(x)}{dx^2} + \left( -\epsilon^2 + \frac{2\alpha^2}{x} - \frac{\tau(\tau-1)}{x^2} \right) R(x) = 0 \quad (76)$$

where

$$\tau = \frac{1}{2} + \sqrt{\alpha^2 + \left( l + \frac{1}{2} \right)^2} \quad \tau(\tau-1) = \alpha^2 + l(l+1) \quad (77)$$

In order to solve this equation with AIM for  $l \neq 0$ , we should transform this equation to the form of Eq.(11). Therefore, the reasonable physical wave function we propose is as follows

$$R(x) = x^\tau e^{-\epsilon x} F(x) \quad (78)$$

If we insert this wave function into the Eq.(76), we have the second-order homogeneous linear differential equations in the following form

$$\frac{d^2 F(x)}{dx^2} = 2 \left( \epsilon - \frac{\tau}{x} \right) \frac{dF(x)}{dx} + 2 \left( \frac{\epsilon\tau - \alpha^2}{x} \right) F(x) \quad (79)$$

which is now amenable to an AIM solution. To apply the AIM, it is required to compare Eq.(79) with Eq.(22). Subsequently, by using Eq. (17), the values of  $\lambda_n(x)$  and  $s_n(x)$  are computed as follows

$$\begin{aligned} \lambda_0(x) &= 2\left(\epsilon - \frac{\tau}{x}\right) \\ s_0(x) &= \frac{2}{x} (\epsilon\tau - \alpha^2) \\ \lambda_1(x) &= \frac{2\tau}{x^2} + \frac{2}{x} (\epsilon\tau - \alpha^2) + \left(2\epsilon - \frac{2\tau}{x}\right)^2 \\ s_1(x) &= 2 (\epsilon\tau - \alpha^2) \left( \frac{2\epsilon}{x} - \frac{2\tau+1}{x^2} \right) \\ \lambda_2(x) &= \frac{4}{x^2} \left( \alpha^2 - \epsilon\tau - \frac{\tau}{x} \right) + \left(2\epsilon - \frac{2\tau}{x}\right) \left[ \frac{6\tau}{x^2} + \frac{4(\epsilon\tau - \alpha^2)}{x} + \left(2\epsilon - \frac{2\tau}{x}\right)^2 \right] \\ s_2(x) &= \frac{4\epsilon\tau - 2\alpha^2}{x^3} + \frac{2\epsilon\tau - 2\alpha^2}{x} \left[ \frac{6\tau}{x^2} + \frac{2(\epsilon(\tau-1) - \alpha^2)}{x} + \left(2\epsilon - \frac{2\tau}{x}\right)^2 \right] \\ &\dots etc \end{aligned} \quad (80)$$

If we use the termination condition of the AIM given in Eq.(19), energy eigenvalues are obtained as follows

$$\frac{s_0}{\lambda_0} = \frac{s_1}{\lambda_1} \Rightarrow \epsilon_0 = \frac{\alpha^2}{\tau} \quad (81)$$

$$\frac{s_1}{\lambda_1} = \frac{s_2}{\lambda_2} \Rightarrow \epsilon_1 = \frac{\alpha^2}{\tau + 1} \quad (82)$$

$$\frac{s_2}{\lambda_2} = \frac{s_3}{\lambda_3} \Rightarrow \epsilon_2 = \frac{\alpha^2}{\tau + 2} \quad (83)$$

$\dots etc$

which can be generalized as

$$\epsilon_n = \frac{\alpha^2}{\tau + n} \quad (84)$$

If one inserts the values of  $\epsilon$ ,  $\tau$ , and  $\alpha$  into equation (84), the ro-vibrational energy spectrum of the Schrödinger equation with the non-central modified Kratzer potential becomes

$$E_{nl} = D - \frac{8\mu a^2}{\hbar^2} D^2 \left[ 1 + 2n + \sqrt{1 + 4 \left( \frac{2\mu a^2 D}{\hbar^2} + l(l+1) \right)} \right]^{-2} \quad (85)$$

where  $n$  and  $l$  are the vibrational and the rotational quantum numbers, respectively.

As indicated in Section III, we can construct the corresponding eigenfunctions by using Eq.(30). Eq.(79) provides Eq.(22) for  $N=-1$ ,  $b=0$ ,  $a=\epsilon$  and  $m=\tau-1$ .

Equation (31) can be written using limit relation as  $b \rightarrow 0$  in the following form

$$\lim_{b \rightarrow 0} {}_2F_1(-n, 1/b + a; c; zb) = {}_1F_1(-n; c; z) \quad (86)$$

$$y_n(x) = (-1)^n C_2(N+2)^n (\sigma)_n {}_1F_1(-n, \sigma; \frac{2a}{N+2} x^{N+2}) \quad (87)$$

Directly solutions  $F_n(x)$  for the eigenvalue problem Eq.(85) can be obtained from Eq.(87) with the substitution  $N=-1$  and  $a=\epsilon$ .

$$F_n(x) = (-1)^n C_2(\sigma)_n {}_1F_1(-n, \sigma; 2\epsilon x) \quad (88)$$

where  $\sigma=2\tau$ , and  $(\sigma)_n = \frac{\Gamma(\sigma+n)}{\Gamma(\sigma)}$ . Consequently, the radial eigenfunction for Schrodinger equation with modified Kratzer potential is

$$R(x) = x^\tau e^{-\epsilon x} (-1)^n C_2(\sigma)_n {}_1F_1(-n, 2\tau; 2\epsilon x) \quad (89)$$

$$R(r) = \left(\frac{r}{a}\right)^\tau e^{-\epsilon \frac{r}{a}} (-1)^n C_2(\sigma)_n {}_1F_1\left(-n, 2\tau; 2\epsilon \frac{r}{a}\right) \quad (90)$$

where  $C_2$  is normalization constant.

We now probe solutions of the angle-dependent Schrödinger equation with the non-central modified Kratzer potential using the same approach. The non-relativistic angular motion of a diatomic molecule of mass  $\mu$  is described by the following equation,

$$\frac{d^2 H(\theta)}{d\theta^2} - \left( \frac{2\mu}{\hbar^2} V(\theta) + \frac{m^2}{\sin^2 \theta} - \frac{1}{2} - \frac{1}{4} \frac{\cos^2 \theta}{\sin^2 \theta} - l(l+1) \right) H(\theta) = 0 \quad (91)$$

If we define as  $l=l'-\frac{1}{2}$  and  $l(l+1)=l'^2-\frac{1}{4}$ , Eq. (91) can be written as

$$\frac{d^2 H(\theta)}{d\theta^2} - \left[ \frac{2\mu\beta/\hbar^2 + m^2 - 1/4}{\sin^2 \theta} + \frac{2\mu\gamma \cos \theta / \hbar^2}{\sin^2 \theta} \right] H(\theta) = -l'^2 H(\theta) \quad (92)$$

This equation can be further arranged as

$$\frac{d^2 H(\theta)}{d\theta^2} - \left[ \frac{\kappa^2 + \eta^2 - 1/4}{\sin^2 \theta} + \frac{2\kappa\eta \cos \theta}{\sin^2 \theta} \right] H(\theta) = -l'^2 H(\theta) \quad (93)$$

with

$$\kappa^2 = \frac{1}{2} \left[ \frac{2\mu\beta}{\hbar^2} + m^2 + \sqrt{(m^2 + \frac{2\mu\beta}{\hbar^2})^2 - \left( \frac{2\mu\gamma}{\hbar^2} \right)^2} \right] \quad (94)$$

$$\eta^2 = \frac{1}{2} \left[ \frac{2\mu\beta}{\hbar^2} + m^2 - \sqrt{(m^2 + \frac{2\mu\beta}{\hbar^2})^2 - \left( \frac{2\mu\gamma}{\hbar^2} \right)^2} \right] \quad (95)$$

Equation (93) can be written in the following form by introducing a new variable of the form  $x = \cos \theta$ ,

$$\frac{d^2 H(x)}{dx^2} + \frac{x}{1-x^2} \frac{dH(x)}{dx} - \left[ \frac{\kappa^2 + \eta^2 + 2\kappa\eta x}{(1-x^2)^2} \right] H(x) = -\frac{l'^2}{1-x^2} H(x) \quad (96)$$

Let the angular wave function be factorized as:

$$H(x) = (1-x)^{(\frac{\kappa+\eta}{2}+1/4)} (1+x)^{(\frac{\kappa-\eta}{2}+1/4)} f(x) \quad (97)$$

Equation (96) reduces to the second-order homogeneous linear differential equation in the following form

$$\frac{d^2 f(x)}{dx^2} = 2 \left( \frac{\eta + (\kappa+1)x}{1-x^2} \right) \frac{df(x)}{dx} + \left( \frac{(\kappa+1/2)^2 - l'^2}{1-x^2} \right) f(x) \quad (98)$$

which is convenient to a AIM solution. In order to find the solution of this equation, it is necessary to compare Eq.(98) with Eq.(11). By means of Eq. (17), the values of  $\lambda_n(x)$  and

$s_n(x)$  are obtained as follows

$$\begin{aligned}
\lambda_0(x) &= \frac{2\eta + (2\kappa + 2)x}{1 - x^2} \\
s_0(x) &= \frac{(\kappa + 1/2)^2 - l'^2}{1 - x^2} \\
\lambda_1(x) &= \frac{(\kappa + 1/2)^2 - l'^2 + 2\kappa + 2}{1 - x^2} + \frac{(2\eta + (2\kappa + 2)x)(2\eta + (2\kappa + 4)x)}{(1 - x^2)^2} \\
s_1(x) &= \frac{((\kappa + 1/2)^2 - l'^2)(2\eta + (2\kappa + 4)x)}{(1 - x^2)^2} \\
\lambda_2(x) &= \frac{2(\eta + (\kappa + 1)x)((\kappa + 1/2)^2 - l'^2 + 6\kappa + 8)}{(1 - x^2)^2} \\
&\quad + \frac{2(\eta + (\kappa + 1)x)((\kappa + 1/2)^2 - l'^2 + 8x^2 + (2\eta + (2\kappa + 2)x)(2\eta + (2\kappa + 8)x))}{(1 - x^2)^3} \\
s_2(x) &= \frac{((\kappa + 1/2)^2 - l'^2)((\kappa + 1/2)^2 - l'^2 + 2(2\kappa + 2))}{(1 - x^2)^2} \\
&\quad + \frac{((\kappa + 1/2)^2 - l'^2)(8x^2 + 6(2\eta + (2\kappa + 2)x)x + (2\eta + (2\kappa + 2)x)^2)}{(1 - x^2)^3} \tag{99}
\end{aligned}$$

... etc

Combining these results with the condition given by Eq.(19) yields

$$\frac{s_0}{\lambda_0} = \frac{s_1}{\lambda_1} \Rightarrow l'^2 = \left(\kappa + \frac{1}{2}\right)^2 \tag{100}$$

$$\frac{s_1}{\lambda_1} = \frac{s_2}{\lambda_2} \Rightarrow l'^2 = \left(\kappa + \frac{3}{2}\right)^2 \tag{101}$$

$$\frac{s_2}{\lambda_2} = \frac{s_3}{\lambda_3} \Rightarrow l'^2 = \left(\kappa + \frac{5}{2}\right)^2 \tag{102}$$

... etc

When the above expressions are generalized, the eigenvalues turn out as

$$l'^2 = \left(\kappa + N + \frac{1}{2}\right)^2, \quad N = 0, 1, 2, \dots \tag{103}$$

Inserting  $\kappa$  and  $l'$  in Eq.(103)

$$l = \sqrt{\frac{\frac{2\mu\beta}{\hbar^2} + m^2 + \sqrt{(m^2 + \frac{2\mu\beta}{\hbar^2})^2 - (\frac{2\mu\gamma}{\hbar^2})^2}}{2}} + N \tag{104}$$

If  $l$  value obtained by Eq.(104) is inserted into energy spectrum of radial part of the Schrödinger equation given by Eq.(85), we find energy spectrum for a diatomic molecule system in the presence of non-central modified Kratzer potential as following,



$$E_{nm} = D - \frac{8\mu D^2 a^2}{h^2} \times \left[ 1 + 2n + \sqrt{1 + 4 \left( \frac{2\mu D a^2}{h^2} + \left( \sqrt{\frac{m^2 + \frac{2\mu\beta}{h^2} + \sqrt{(m^2 + \frac{2\mu\beta}{h^2})^2 - (\frac{2\mu\gamma}{h^2})^2}}}{2} + N \right) \left( \sqrt{\frac{m^2 + \frac{2\mu\beta}{h^2} + \sqrt{(m^2 + \frac{2\mu\beta}{h^2})^2 - (\frac{2\mu\gamma}{h^2})^2}}}{2} + N + 1 \right) \right)} \right]^{-2} \quad (105)$$

This eigenvalue equation obtained by using the asymptotic iteration method is the same as the 63. As similar to radial wavefunction, angular wavefunction can be found by using Eq.(30). The advantage of the asymptotic iteration method is that it gives the eigenvalues directly by transforming the second-order differential equation into a form of  $y'' = \lambda_0(r)y' + s_0(r)y$ . The wave functions are easily constructed by iterating the values of  $s_0(r)$  and  $\lambda_0(r)$ . The method presented in this study is a systematic one and puts no constraint on the potential parameter values involved.

## VI. INTERPRETATION OF THE RESULTS

In comparison with the eigenvalue equation (49) of the modified Kratzer potential, the eigenvalue equations given by equations (63 and 105) have the correction due to the angle-dependent (non-central) part of the modified Kratzer potential, given by equation (32). This correction has two dependencies: First one is due to the values of the constants  $\beta$  and  $\gamma$  in the non-central part of the potential. Different values of the  $\beta$  and  $\gamma$  change the shape and the depth of the potential which affects the values of the energy eigenvalues. The second one is because of the orbital angular momentum quantum number  $l$  given by equation (62). It is known that the orbital angular momentum quantum number  $l$  is a good quantum number and it is a constant of motion for the central potentials such as the modified Kratzer potential. On the other hand, for the non-central modified Kratzer potential, it is no longer a constant of motion and its value is determined in terms of the constants  $\beta$  and  $\gamma$  as well as  $n$  and  $m$  quantum numbers as given in equation (62). This is the effect of the non-central part of the potential which modifies the  $l$  values. For  $\beta=\gamma=0$ , the non-central modified Kratzer potential reduces to the modified Kratzer and they should give the same energy eigenvalues for the same  $l$  values. For the modified Kratzer potential,  $l$  is a constant of the motion and takes the values  $l=0,1,2,\dots$ , but for the non-central modified Kratzer potential, it is determined from equation (62). Therefore, they give the same energy eigenvalues as long

as the following condition is satisfied: the  $l$  value of the modified Kratzer potential is equal to  $(n + m)$  of the non-central modified Kratzer potential for  $\beta=\gamma=0$ . By comparing the eigenvalue equation ( $E_{nm}$ ) for the non-central Kratzer potential given by equations (63 and 105) with the eigenvalue equation ( $E_{nl}$ ) for the modified Kratzer potential given by equation (49), we note that the effect of the non-central part is small for the small values of  $\beta$  and  $\gamma$  constants, but the difference becomes apparent when they have large values. In order to show this, the difference between the eigenvalues of the modified Kratzer and non-central modified Kratzer potentials is demonstrated in comparison with each other in Table II for different  $n$ ,  $l$  and  $m$  quantum numbers.

## VII. CONCLUSION

In this study, we have calculated the exact bound-state energy eigenvalues and the corresponding eigenfunctions of the new exactly solvable non-central modified Kratzer potential by using two different methods. Both NU and AIM methods generate the same results. In comparison with the NU method, AIM puts no constraint on the potential parameter values involved. Therefore, AIM is more systematic than the NU method in solving such second-order differential equations.

In our study, we have determined the effect of the non-central term on the bound-state energy eigenvalues explicitly. The energy eigenvalue equations for the modified and non-central modified Kratzer potentials are given by equation (49) and equations (63 and 105), respectively. In comparison with the eigenvalues of the modified Kratzer potential, the effect due to the angle-dependent part of the non-central potential on the energy eigenvalues is shown for the *CO* molecule in Table II. The correction is very small for the small values of  $\beta$  and  $\gamma$  in the angle dependent part of the potential. However, the difference becomes apparent for the values of  $\beta=\gamma=1$  and over. In order to examine this effect, we have plotted the shape of the modified Kratzer and non-central modified Kratzer potential in Figure 1 for different values of  $\beta$  and  $\gamma$ . We perceive from this figure that the sum of the modified Kratzer and centrifugal potentials with  $l=50$  gives almost the same shape for the non-central modified Kratzer potential with  $\beta=\gamma=1$ . That is, the angle-dependent part behaves like the centrifugal barrier and as it is clearly seen in Figure 1, it reduces the depth of the potential pocket, which effects the bound-state energy eigenvalues.

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- [1] F. Cooper, A. Khare and U. Sukhatme, Phys. Rep. **251** (1995) 267.
- [2] D. A. Morales, Chem. Phys. Letters **394** (2004) 68.
- [3] B. Gönül, I. Zorba, Phys. Lett. A **269** (2000) 83.
- [4] A. F. Nikiforov and V. B. Uvarov, **Special Functions of Mathematical Physics**, Birkhäuser, Basel, (1988).
- [5] H. Egrifes, D. Demirhan and F. Büyükkilic, Phys. Scripta **59** (1999) 90.
- [6] M. Aktas, R. Sever, J. Phys. Math. Chem. **37(2)** (2005) 139.
- [7] F. Yasuk, C. Berkdemir and A. Berkdemir, J. Phys. A: Math. Gen. **38** (2005) 6579.
- [8] C. Berkdemir, A. Berkdemir and J. Han, Chem. Phys. Lett. **417** (2006) 326.
- [9] H. Ciftci, R. L. Hall and N. Saad, J. Phys. A: Math. Gen. **36** (2003) 11807.
- [10] H. Ciftci, R. L. Hall and N. Saad, J. Phys. A: Math. Gen. **38** (2005) 1147.
- [11] I. Boztosun, M. Karakoc, F. Yasuk and A. Durmus, J. Math. Phys. **47** (2006) 062301.
- [12] O. Bayrak and I. Boztosun, J. Phys. A: Math. Gen. **39** (2006) 6955.
- [13] M. Aygun, O. Bayrak and I. Boztosun, J. Phys. B: At. Mol. Opt. Phys. **40** (2007) 537.
- [14] C. L. Pekeris, Phys. Rev. **45** (1934) 98.
- [15] S. Flügge, **Practical Quantum Mechanics** Vol. I, Springer, Berlin, (1994).
- [16] A. Kratzer, Z. Phys. **3** (1920) 289.
- [17] R. J. Le Roy and R. B. Bernstein, J. Chem. Phys. **52** (1970) 3869.
- [18] E. Fues, Ann. Physik **80** (1926) 367.
- [19] L. E. Sutton, **Tables of Interatomic Distances and Configuration in Molecules and Ions**, Chem. Soc. of London, (1958).
- [20] G. Szego, *Orthogonal Polynomials* (American Mathematical Society, New York, 1939).

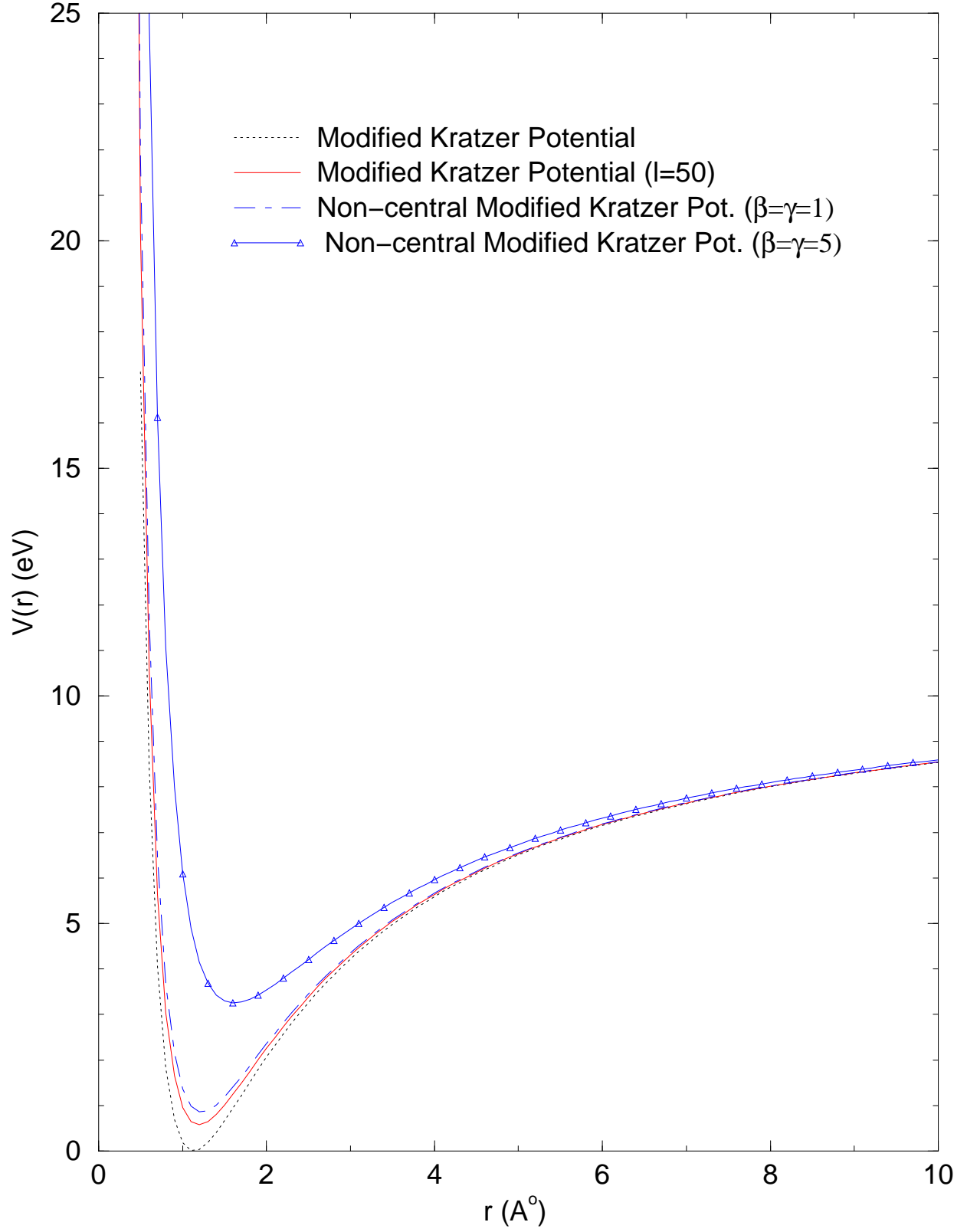


FIG. 1: Comparison of the modified Kratzer and non-central modified Kratzer potentials ( $\theta = 30^\circ$ ) for different  $\beta$  and  $\gamma$  values for the  $CO$  diatomic molecule.

Molecule	$D_e(\text{eV})$	$a$ (in $\text{\AA}^0$ )	$\mu$ (in amu)
<i>CO</i>	10.84514471	1.1282	6.860586

TABLE I: Reduced mass and spectroscopical properties of the *CO* diatomic molecule in the ground state [19].

TABLE II: Comparison of the eigenvalues of the modified Kratzer ( $E_{nl(K)}$ ) and non-central modified Kratzer ( $E_{nm(NC-K)}$ ) potentials for different  $n$ ,  $l$  and  $m$  values with  $\beta = \gamma = 0.0, 0.1, 1.0$  and  $5.0$  values for the *CO* diatomic molecule, calculated by using equations (49), (63) and (105).

$n$	$l$	$m$	$E_{nl(K)}$		$E_{nm(NC-K)}$			
					$\beta = \gamma = 0.0$	$\beta = \gamma = 0.1$	$\beta = \gamma = 1.0$	$\beta = \gamma = 5.0$
0	0	0	0.050753	0.050753	0.050753	0.092637	0.436157	1.717889
	1	1	0.051227	0.051227	0.051227	0.095893	0.445310	1.733400
	2	2	0.052175	0.052175	0.052175	0.099399	0.454672	1.749028
	3	3	0.053596	0.053596	0.053596	0.103170	0.464246	1.764773
1	0	0	0.151080	0.151547	0.151547	0.198791	0.549209	1.826511
	1	1	0.151547	0.152482	0.152482	0.202234	0.558423	1.841886
	2	2	0.152482	0.153883	0.153883	0.205932	0.567844	1.857376
	3	3	0.153883	0.155751	0.155751	0.209899	0.577475	1.872981
2	0	0	0.250015	0.251397	0.251397	0.303835	0.660838	1.933480
	1	1	0.250475	0.252779	0.252779	0.307458	0.670109	1.948719
	2	2	0.251397	0.254621	0.254621	0.311342	0.679584	1.964071
	3	3	0.252779	0.256923	0.256923	0.315498	0.689268	1.979537
3	0	0	0.347582	0.350309	0.350309	0.407780	0.771065	2.038826
	1	1	0.348037	0.352125	0.352125	0.411577	0.780387	2.053929
	2	2	0.348946	0.354396	0.354396	0.415639	0.789913	2.069144
	3	3	0.350309	0.357118	0.357118	0.419978	0.799645	2.084470